

Supplementary Materials: ^{96}Zr tracer diffusion in AZrO_3 (A = Ca, Sr, Ba)

Rokas Sažinas ^{1,2}, Isao Sakaguchi ², Mari-Ann Einarsrud ¹ and Tor Grande ^{1,*}

¹ Department of Materials Science and Engineering, NTNU Norwegian University of Science and Technology, NO-7491 Trondheim, Norway; rokas.sazinas@gmail.com (R.S.); mari-ann.einarsrud@ntnu.no (M.A.E.); grande@ntnu.no (T.G.)

² Research Center for Functional Materials, National Institute for Materials Science, Tsukuba 305-0044, Ibarki, Japan; sakaguchi.isao@nims.go.jp

* Correspondence: grande@ntnu.no

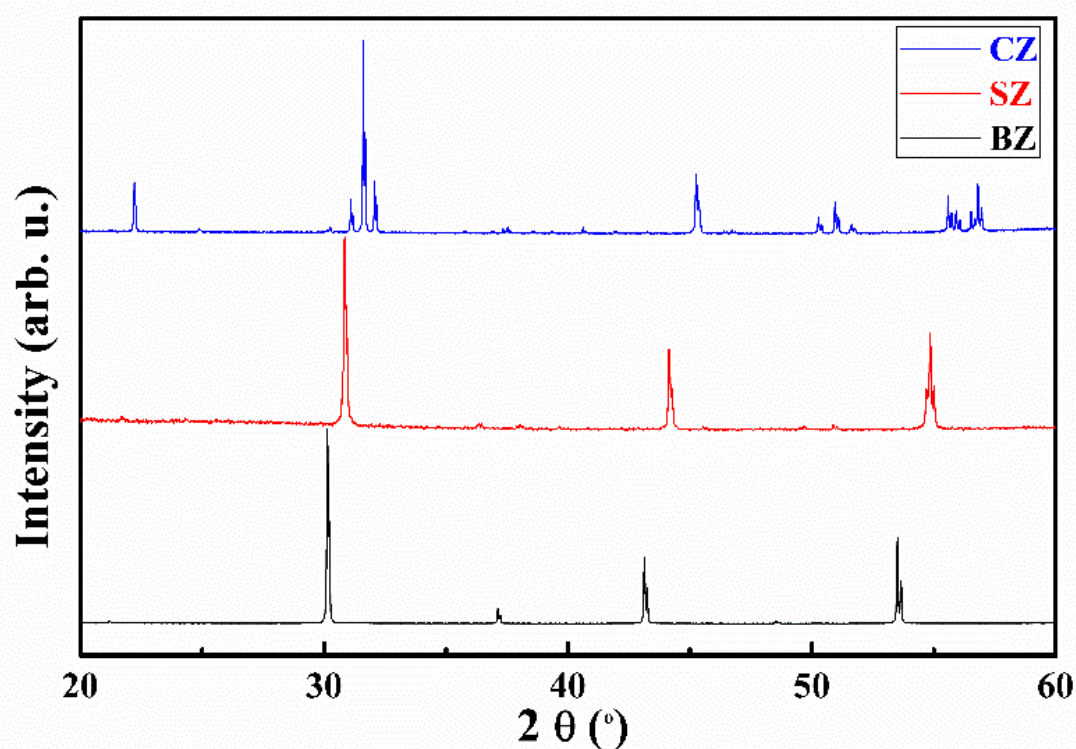


Figure S1. XRD results for sintered CaZrO_3 (CZ), SrZrO_3 (SZ) and BaZrO_3 (BZ) materials.

Table S1. Summary of the sintering results and Rietveld refinement of the ceramics.

Material	Synthesis	Sintering	Grain size (μm)	Parameters*	Crystallite size (nm)	R_{wp}	A/B (Rietveld)	Relative density (%)
BaZrO ₃ (BZ)	Spray pyrolysis	+SacPow* 600 °C/h, 1600 °C, 10 h, air	1.1±0.1	Cubic <i>Pm-3m</i> a = 4.193 Å V = 73.736 Å ³ ρ_{th} = 6.228 g/cm ³	94.59	7.67	0.971	97±1
SrZrO ₃ (SZ)	SSR, 1200 °C, 5 h, air	700 °C/h, 1600 °C, 10 h, air	5.2±0.1	Orthorhombic <i>Pbnm</i> a = 5.797 Å b = 5.824 Å c = 8.209 Å V = 277.152 Å ³ ρ_{th} = 5.437 g/cm ³	108.07	10.74	0.948	96±2
CaZrO ₃ (CZ)	Molten salt (MSS)	700 °C/h, 1550 °C, 2 h, air	10.5±0.2	Orthorhombic <i>Pnma</i> a = 5.763 Å b = 8.023 Å c = 5.596 Å V = 258.68 Å ³ ρ_{th} = 4.604 g/cm ³	113.35	10.04	0.937	98±1

*Errors for refined cell parameters <0.0001