

## HIGH TEMPERATURE X-RAY POWDER DIFFRACTION STUDY OF PHASE TRANSFORMATIONS IN SrZrO<sub>3</sub>

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SrZrO<sub>3</sub> is one of several ABO<sub>3</sub>-type oxides that adopt the orthorhombic GdFeO<sub>3</sub>-type structure under ambient conditions. At higher temperatures there are a series of structural transitions leading to the cubic perovskite structure. These transformations were recently characterized using high temperature neutron diffraction with the sample in vacuum, and three phase transitions were reported: orthorhombic (Pnma) → orthorhombic (Cmcm) → tetragonal (I4/mcm) → cubic (Pm-3m).

In the present study, the high temperature phase transitions of SrZrO<sub>3</sub> have been studied using X-ray powder diffraction. The much faster data acquisition rate achievable on the Philips X'Pert Pro XRD instrument compared to the prior neutron diffraction study enabled time-resolved diffraction analysis of the structural changes. In addition to reproducing the vacuum conditions, the phase equilibria was examined in air and oxygen atmospheres using an Anton Paar high temperature stage. The Rietveld data analysis method was employed using the refined structure data from the neutron study as a starting model for the X-ray structure data.

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