Synchrotron XRD Study of ZrO_2-CeO_2 Nanopowders Synthesised by Gel-combustion

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Zirconia-ceria solid solutions are being widely investigated due to their excellent mechanical and catalytic properties. For example, these materials are extensively used as promoters in three-way catalysts.

In this work, the crystal structure of nanocrystalline ZrO_2-CeO_2 solid solutions, synthesised by a pH-controlled nitrate-glycine gel-combustion process, has been studied by using a high-intensity synchrotron X-ray diffractometer (D12A-XRD1 beamline of the LNLS, Brazilian Light Facility). Several weak Bragg peaks of the tetragonal phase, which correspond to forbidden reflections in the case of a perfect cubic fluorite structure, were detected. By determining the integrated intensity of the strongest of these reflections, (112), as a function of the CeO_2 content, the tetragonal-cubic phase compositional boundary was established to be at (85±5) mol% CeO_2. For a CeO_2 content up to (68±2) mol%, we identified a tetragonal phase with $c/a > 1$, whereas, in the range between 68 and 85 mol% CeO_2, the existence of a tetragonal phase with $c/a = 1$ and oxygen anions displaced from their ideal positions in the cubic phase (keeping the tetragonal symmetry) was verified. Finally, solid solutions with CeO_2 contents higher than 85 mol% exhibit the cubic fluorite-type phase.

Keywords: synchrotron powder diffraction, zirconia-ceria, nanocrystalline materials