

X-ray and neutron diffraction analysis of Ca-Sr-Ti-Fe-O compounds

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CaTi_yFe_{1-y}O_{3-δ}, SrTi_yFe_{1-y}O_{3-δ} and Ca_{0.5}Sr_{0.5}Ti_yFe_{1-y}O_{3-δ} (y~0.65) compounds were synthesized by the polymeric precursor technique and by the ceramic route. The resins resulting from the chemical synthesis were calcined in the 400-1000°C range producing powders with different average particle sizes, evaluated by the laser scattering technique. Room temperature and *in situ* high temperature (θ-θ Bragg-Brentano configuration up to 1200°C with Anton Paar high temperature sample chamber and Braun position sensitive detector) X-ray diffraction, high resolution X-ray diffraction as well as room temperature neutron diffraction experiments (with improved data collection by position sensitive detectors) were carried out in powders heat treated for several hours to increase the average crystallite sizes. Rietveld analyses were performed for structural phase evaluation. Lattice parameter determinations show the partial substitution of Ca²⁺ for Sr²⁺, and the perovskite ABO₃ cubic/orthorhombic structures.

Keywords: calcium strontium titanate, X-ray diffraction, neutron diffraction, Rietveld analysis.

Work supported by CNEN, FAPESP and CNPq.

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