



Structural Investigations of $(\text{Ca},\text{Sr})(\text{Zr},\text{Sn})\text{O}_3$ Perovskite Compounds

H. Larguem, M. Tarrida, S. Rossano and M. Madon

Lab. des géomatériaux, Univ. de Marne la Vallée, CNRS FRE2455
5 Bd Descartes, Champs/Marne
77454 Noisy-Champs cedex 2, France

$(\text{Ca}_x,\text{Sr}_{1-x})\text{ZrO}_3$ and $\text{Ca}(\text{Sn}_x,\text{Zr}_{1-x})\text{O}_3$ solid solutions have been synthesized by solid-state reaction at high temperature. Compounds have been studied by powder X-ray diffraction and Raman Spectroscopy.

Diffraction data allow to study the evolution of the distortion of the ABO_3 perovskite structure with cation substitution on A and B-sites. It is shown that distortion, characterised by Φ , the tilt angle of the BO_6 octahedron, slightly increases with increasing x content in $\text{Ca}(\text{Sn}_x,\text{Zr}_{1-x})\text{O}_3$ compounds and strongly decreases with increasing x content in $(\text{Ca}_x,\text{Sr}_{1-x})\text{ZrO}_3$ compounds. Such results are discussed in view of the relative A and B cation sizes.

Raman data show that vibrational spectra are strongly affected by the cation substitution on the A-site; most of the vibrational modes increase with increasing x content in $(\text{Ca}_x,\text{Sr}_{1-x})\text{ZrO}_3$ compounds, i.e. with the decreasing mean size of the A-cation. On the other hand, the cation substitution on B-sites, slightly affect the spectra; it is shown that only the mode located at about 280 cm^{-1} significantly decreases with increasing x content in $\text{Ca}(\text{Sn}_x,\text{Zr}_{1-x})\text{O}_3$ compounds, i.e. with the decreasing mean size of the B-cation.

Such results are used to predict the location of trivalent cations (Nd^{3+} and Al^{3+}) on A- or B-site, in the perovskite structure.