Keywords: CaO–La2O3–TiO2 ternary system, Structure relations, Perovskites, X-Ray powder diffraction, Rietveld refinement

MS16-P3 Sol–gel synthesis of double perovskite quaternary tellurium-containing metal oxides: Ba_2NiTeO_6, Ba_2CoTeO_6

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Interest in double perovskite $A_2B'B''O_6$ structures comes from the discovery of its colossal magnetoresistance properties exhibited at room temperature by Sr_2FeMoO_6.[1] Later it was discovered that perovskites can also act as electrode materials in solid oxide fuel cells (SOFCs),[2,3] and transducers and memories,[4,5] indicating why it is important to invest time to fully understand the nature of their physical and chemical characteristics.

Highly crystalline double perovskite Ba_2NiTeO_6 and Ba_2CoTeO_6 have been prepared via novel sol-gel route using citric acid as chelating agent. Both materials have been studied by X-ray diffraction (XRD), scanning electron microscope (SEM), transmission electron microscopy (TEM), and SQUID magnetic measurements. As obtained XRD patterns are carefully analyzed by the Rietveld method using programs X'Pert Highscore Plus and FULLPROF.[6,7]

It was found that at room temperature Ba_2NiTeO_6 crystallizes in space group *R*-3*m* with a =5.7965(4) Å, c = 28.600(3) Å. Ba_2CoTeO_6 has been refined in the space group *R*-3*m*; a = 5.8003(2) Å, c = 14.2672(5) are showing trigonal perovskite structure. Average crystallite size is 44 nm for Ba_2NiTeO_6 and 104 nm for Ba_2CoTeO_6, respectively.

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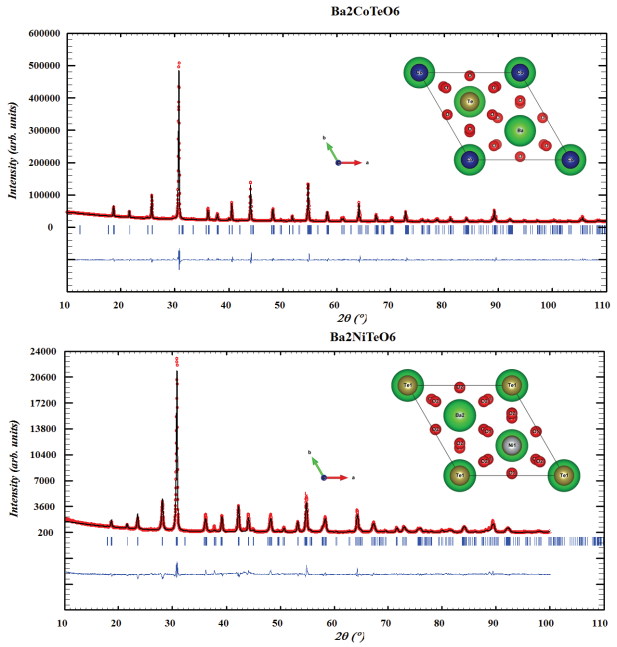

Figure 1. XRD Refinement for a) Ba_2CoTeO_6 and b) Ba_2NiTeO_6 made by FULLPROF program. Inset is 3D visualization program for structural models made by Vesta software.

Keywords: double perovskite, sol-gel synthesis, XRD refinement

MS16-P4 Phase transitions in relaxor ferroelectric materials with tungsten bronze type structures

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Ferroelectric materials are essential for modern electronic applications, from consumer electronics to sophisticated technical instruments. Relaxor ferroelectric materials provide the advantage of high dielectric constants over broad temperature ranges not seen in traditional ferroelectrics. Tungsten bronze type compounds have been shown to display a variety of industrially relevant optical and electronic properties amongst others. There is a fundamental relationship between the physical properties displayed by ferroelectrics and the crystal structures in which they form. Of particular interest are compositions and temperatures near phase transition. These are important because near phase transitions, particularly morphotropic phase transitions, physical properties are often dramatically enhanced.[1,2] This work focuses on the structural investigation of tungsten bronze type relaxor ferroelectric materials in the system $Ba_xSr_{3-x}Ti_{1-y}Zr_yNb_4O_{15}$ ($0 \leq x \leq 3$; $0 \leq y \leq 1$). A combination of X-ray, neutron (ToF and constant wavelength) and electron diffraction were employed to map the room temperature phase diagram. In addition, morphotropic phase boundary compositions were determined accurately. Variable temperature synchrotron X-ray diffraction studies were utilised to further explore the phase diagram for non-ambient conditions. Temperature dependent phase transitions were determined and the relationship between composition and transition temperature analysed. Structural models used in this work resulted from Rietveld refinements against powder diffraction data. This work will shed light on new lead free relaxor ferroelectric materials.

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