XRD AND VIBRATIONAL SPECTROSCOPY INVESTIGATION OF $BaTi_{1-x}Sn_xO_3$ SOLID SOLUTIONS

Lj. Veselinović[a*], M. Mitrić[b], S. Marković[a], D. Uskoković[a]

[a]Institute of Technical Sciences of the Serbian Academy of Sciences and Arts,
[b]The Vinča Institute of Nuclear Sciences, Belgrade, Serbia

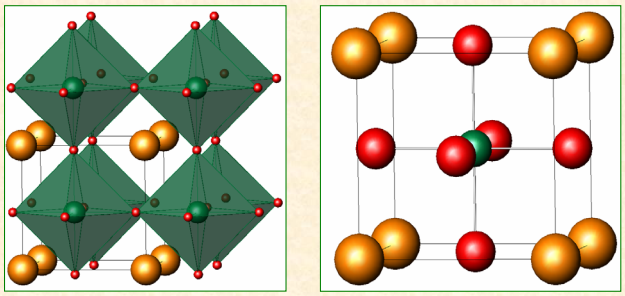

***Fig. 1**. Representation of ideal cubic crystal structure of perovskites along b-axis. The corner-linked BX_6 octahedra (green) and centrally located A cations (gold). The oxygen is present as a red spheres.*

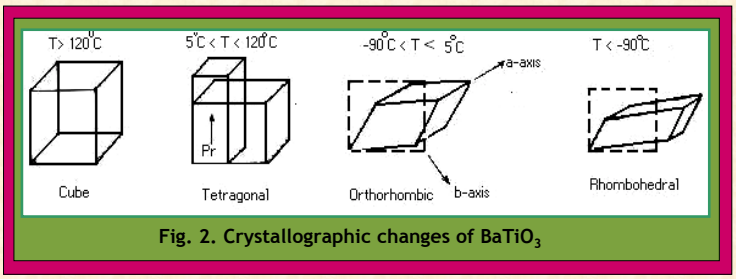

Fig. 2. Crystallographic changes of $BaTiO_3$

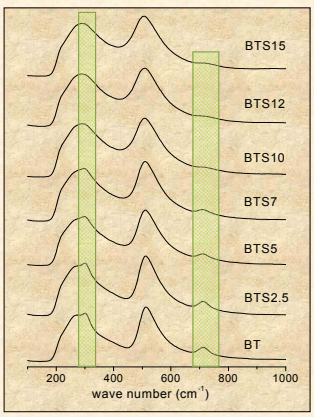

Fig. 3 Raman spectra of BTS samples

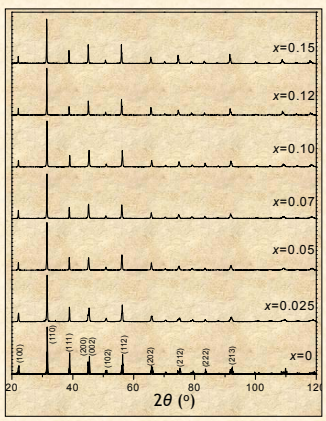

Fig. 4 XRD patterns of BTS powders

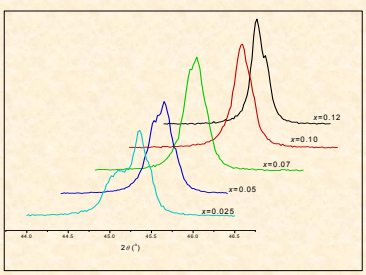

Fig. 5 The changes in the (200) reflection with x =0.025, 0.05, 0.07, 0.10 (tetragonal phases) and 0.12 (cubic phase).

Introduction

The perovskites ABX_3 represent wide group of minerals which are very important due to their excellent electrophysical properties. Unique electrical properties of perovskites are due to their crystal structure, which makes them very applicable in different area of industry. The ideal crystal structure of the perovskites is cubic with space group symmetry *Pm*3*m*. The structure can be described as a threedimensional network of regular corner-linked BX_6 octahedra, the *B* cations being at the centre of these octahedra and the *A* cations being centrally located in the spaces between them (Fig. 1). Due to the high stability and flexibility of the perovskites structure a wide range of substitution of cations *A* and *B*, as well as the anions, are possible.

The variety of crystal structure is caused by phase transitions, which can occurs as a response to changes in temperature, pressure, and composition (Fig. 2).

The $BaTiO_3$ materials have the perovskite crystal structural. They have a great application in electronic industry as a dielectric and ferroelectric materials. The BaTiO3 doped with Sn is important for practical application in ceramic capacitors as well as in functionally graded materials.

Materials and methods

In this study the structure of barium titanate stannate (BTS) $BaTi_{1-x}Sn_xO_3$ (x = 0, 0.025, 0.05, 0.07, 0.10, 0.12, 0.15) solid solutions was investigated. The BTS powders, with different Sn amount were synthesized by solid-state reaction technique. The structural investigations of the BTS samples were done at room temperature using an X-ray powder diffraction and Raman spectroscopy measurements. The XRD patterns were obtained on a Philips PW-1050 automatic diffractometer using $CuK\alpha_{1,2}$ radiation at 40 kV and 20 mA. The diffraction measurements were made over scattering angle 2θ from 20 to 120° with a step of 0.02° and a counting time of 15 s.

Raman spectroscopy investigations were carried out by a Raman System R-2001 Spectrometer, equipped with a linear silicon CCD detector. The samples were excited using a red solid-state diode laser at 785 nm. The Raman spectra were recorded in the frequency interval 200- 2000 cm^{-1}.

Results

The X-ray powder diffraction analysis confirmed pure perovskite phase in all samples, irrespective of Sn content in the powders. It can be observed that diffraction maximums are shifted towards lower 2θ angles as a consequence of replacement Ti^{4+} -ions by larger Sn^{4+}-ions. The diffraction data clearly indicate on changes of crystal structure with increasing Sn amount in the powders. The doubled 2 0 0 reflections at ~ 45° 2θ typical for tetragonal perovskite structure becomes one, corresponding cubic perovskite crystal structure (Fig. 5).

The phase transformation from tetragonal to cubic crystal structure was confirmed by Raman spectroscopy (Fig. 3). It is evident that intensities of the bands at about 300 i 711 cm^{-1} decrease with increase Sn content which indicate on phase transitions in the perovskite crystal strukture.

Conclusion

The barium titanate stannate (BTS) $BaTi_{1-x}Sn_xO_3$ (x = 0, 0.025, 0.05, 0.07, 0.10, 0.12, 0.15) solid solutions was investigated by X-ray powder diffractin and Raman spectroscopy. It was confirmed that increasing of Sn content in the perovskite structure results in reduction of the symmetry from cubic to tetragonal.