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STRUCTURE PECULIARITIES AND ELECTROPHYSICAL PROPERTIES OF $(1-x)BaTiO_3$-$xNa_{0.5}Bi_{0.5}TiO_3$ SOLID SOLUTIONS

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In recent years, materials based on $(1-x)BaTiO_3$–$xNa_{0.5}Bi_{0.5}TiO_3$ solid solutions have aroused great interest [1]. This interest is due to the fact that lead-free materials with positive temperature coefficient of resistance (PTCR) and with piezoelectric properties can be developed on their basis. However, literature data relating to this system is controversial. In particular, some authors report that $(1-x)BaTiO_3$–$xNa_{0.5}Bi_{0.5}TiO_3$ solid solutions are single-phase and have tetragonal structure (space group $P4mm$) in the range $0 \le x < 0.9$, whereas in the range $0.9 < x \le 1$ they have rhombohedral structure (space group $R3c$) [2]. But other authors suggest that there is a morphotropic phase boundary (MPB) at $x \cong 0.95$ [3]. Thus, it was important to clarify the conditions of MPB formation during synthesis by solid state reactions; to determine the unit cell parameters of the solid solutions formed in the system; to find additional phases or to be sure that a single-phase product is formed. In addition, an explanation of the change in the electrophysical properties of materials in the MPB area is required.

The aim of this work was to study the structure peculiarities and the electrophysical properties of $(1-x)BaTiO_3$–$xNa_{0.5}Bi_{0.5}TiO_3$ solid solutions.

Bulk samples of $(1-x)BaTiO_3$–$xNa_{0.5}Bi_{0.5}TiO_3$ were prepared by the solid-state reaction technique. The phase purity and the crystal structure were examined by powder X-ray diffraction. The concentration ranges of the formation of solid solutions have been determined. It has been found that ceramics with x values near zero or near unity can be sintered at 1240-1270°C, while in the range $0.6 \le x \le 0.9$, high-density ceramics can be sintered at temperatures below 1220°C. Unit cell parameters, interatomic distances and bond angles were deduced from the Rietveld refinement of XRPD data. The permittivity and dielectric loss tangent have been investigated in wide frequency and temperature ranges. The maximum value of permittivity has been shown to vary nonlinearly with x. At $x = 0.9$, the maximum of dielectric constant is observed, which can be accounted for by the fact that MPB is formed. Therefore, the materials with x near 0.9 are of interest as piezoelectrics. A correlation between electrophysical properties and unit cell parameters has been established. The main peculiarities of the variation of the phase transition parameters with crystal parameters have been determined.

At $0 \le x < 0.2$, the tetragonal distortion (c/a), which causes the ferroelectric properties of the $(1-x)BaTiO_3$–$xNa_{0.5}Bi_{0.5}TiO_3$ solid solution, does not change significantly. This fact shows a considerable potential of their investigation as a basis for the creation of PTCR elements. A comparative analysis of the PTCR properties of elements based on the lead-free $(1-x)BaTiO_3$–$xNa_{0.5}Bi_{0.5}TiO_3$ system and the lead-containing $(1-x)BaTiO_3$–$xPbTiO_3$ system has been performed.

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[3] J.-R. Gomah-Pettry, S. Saïd, P. Marchet, J.-P. Mercurio, *J. Eur. Ceram. Soc.* 24 (2004) 1165-1169.