SOME IDEAS ON MODELING THE TRANSPORT PROCESSES
IN THE SYSTEM Bi$_2$O$_3$-TiO$_2$-Nd$_2$O$_3$-SiO$_2$

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Abstract: In our previous studies bismuth-titanate ceramics was synthesized by melt quenching method in the system Bi$_2$O$_3$-TiO$_2$-Nd$_2$O$_3$-SiO$_2$ at temperature range 1250 – 1500 °C. The phase composition of the obtained materials was determined by X-ray diffraction analysis and energy dispersive spectroscopy. Different microstructures observed by scanning electron microscopy were proved to depend on the composition. Conductivity, dielectric losses and relative permittivity were studied depending on the composition. The aim of this work is to present some ideas for study of composite materials in the system Bi$_2$O$_3$-TiO$_2$-SiO$_2$-Nd$_2$O$_3$ using mathematical modeling of their properties. The relationship between content of the observed phases (Bi$_2$Ti$_2$O$_7$, Bi$_4$Ti$_3$O$_{12}$, Bi$_2$TiO$_{20}$, and δ-Bi$_2$O$_3$) and the electrical and dielectric properties will be followed.

Keywords: bismuth titanate ceramics, melt quenching, electrical characteristics, microstructure, mathematical modeling

I. INTRODUCTION

Aurivillius family oxides including Bi$_4$Ti$_3$O$_{12}$ were of grate interest with their potential use for electronic applications with high temperature piezoelectric properties (high Curie temperature) [1, 2]. Applications of bismuth-based ferroelectrics were strongly influenced by the method of preparation [3-18]. S. Kunej et all. [19] studied the phase-formation in the system Bi$_2$O$_3$-TiO$_2$-Nd$_2$O$_3$ and formation of solid-solution of Bi$_{4-x}$Nd$_x$Ti$_2$O$_{12}$.

The previously obtained samples in the systems Bi$_2$O$_3$-TiO$_2$-SiO$_2$ and Bi$_2$O$_3$-TiO$_2$-SiO$_2$-Nd$_2$O$_3$ [20-23] are determined as polycrystalline ceramics or glass-ceramics. According to the X-ray data [23], several phases are identified including Bi$_2$Ti$_2$O$_7$, Bi$_4$Ti$_3$O$_{12}$, Bi$_2$TiO$_{20}$ and δ-Bi$_2$O$_3$. Electrical characteristics were studied by: (1) Arrhenius plot of the conductivity in dependence on the temperature, (2) the temperature dependence of the dielectric constant and (3) the temperature dependence of dielectric losses. It was established that increasing the Nd$_2$O$_3$ and SiO$_2$ content up to 10 mol % of leaded to increase the activation energy of Nd$_2$O$_3$ and to decrease the activation energy of SiO$_2$ [23]. Co-addition of SiO$_2$ and Nd$_2$O$_3$ up to 5 mol % caused d an activation energy of 1 eV, whereas the co-addition of both oxides up to 10 mol % - close to 1.7 eV. The results were obtained in the temperature range of (1.2 – 2).10$^3$ K$^{-1}$ [23]. A decreasing of the dielectric constant ($\varepsilon_r$) was observed when decreasing SiO$_2$ content from 20% to 10% [23].
Some methods for calculation of the dielectric properties of solid-solutions and poly-phase composites of dielectrics were reported [24]:

1. Non-homogeneous dielectric could be defined as two or more dielectrics in series.
2. Non-homogeneous dielectric could be defined as two or more dielectrics in parallel.
3. Dielectric, which is a complex heterogeneous mixture of one or more components dispersed as small grains in the volume: the equation of Leyendecker and Roth were used.
4. Complex dielectric, defined as a matrix mixture: the equation of Maxwell and Wagner was proposed.
5. Matrix mixture in which dispersed phase has a high conductivity: the equation of Bruggeman was used.

Our previous results and mentioned above mathematical models motivated us to search methods for mathematical modeling to predict the properties according to their composition.

II. ALGORITHM OF THE RESEARCH

To make mathematical model of the charge behavior of the system Bi$_2$O$_3$-TiO$_2$-SiO$_2$-Nd$_2$O$_3$, we need to:

1. Make a structure model (phase formation, defects and defect mobility).
2. Make a model for charge transport (for dielectric losses, dielectric permittivity and relaxation time).

These two points are characterized with the next steps:

- Choice of a physical model – choice of the well know physical model according to the number and type of phase components;
- Formalization – choice of the model parameters;
- Choice of the mathematical procedures;
- Creation of the model and make virtual experiments;
- Make statistical calculation and validation with real experimental data.

III. CONCLUSION

Analysis will be made of the resulting models in order to be used in the development of experimental procedures for the synthesis system Bi$_2$O$_3$-TiO$_2$-SiO$_2$-Nd$_2$O$_3$. Calculation procedures will aim to quantify the content of different phases.

This study could be treated as a step in the creation of new functional materials.

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REFERENCES


