The Serbian Society for Ceramic Materials
Institute for Multidisciplinary Research (IMSI), University of Belgrade
Institute of Physics, University of Belgrade

Center of Excellence for the Synthesis, Processing and Characterization of Materials for use in Extreme Conditions "CEXTREME LAB" - Institute of Nuclear Sciences "Vinča", University of Belgrade

Faculty of Mechanical Engineering, University of Belgrade

Center for Green Technologies, Institute for Multidisciplinary Research, University of Belgrade

Faculty of Technology and Metallurgy, University of Belgrade Faculty of Technology, University of Novi Sad

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P-43

## THEORETICAL AND EXPERIMENTAL STUDY OF POLYCRYSTALLINE PHASES OBTAINED BY THE NANOMETRIC ZnTiO<sub>3</sub> POWDER SINTERING

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In this study we have combined two research methods: structure prediction of ZnTiO<sub>3</sub> using computational SPuDS software, and the characterization of binary oxides obtained from ZnO TiO<sub>2</sub> system. Pure nanosized ZnTiO<sub>3</sub> (99.5%), was compacted in cylindrical shape specimens by uniaxial double sided compaction and then sintered in air atmosphere in a dilatometric device [1,2]. One compact was sintered up to 915 °C to retain metastabile ZnTiO3 and held 5 minutes on that temperature, and another one at the same conditions, but now up to 970 °C to induce phase transition and to obtain stabile Zn<sub>2</sub>TiO4 and TiO<sub>2</sub> according to phase diagram [2]. Reheated samples obtained at different characteristic temperatures in air were analyzed by X-ray diffraction (XRD). The infrared attenuated total reflectivity measurements confirmed XRD results. In order to estimate theoretical stability of these perovskite structure, Goldschmidt tolerance factor Gt and global instability index GII were calculated. Furthermore, the Ti valence states were determined by bond valence calculations (BVC). Also, we have investigated the formation of new phases (Zn<sub>2</sub>Ti<sub>3</sub>O<sub>8</sub>, TiO<sub>2</sub> and Zn<sub>2</sub>TiO<sub>4</sub>) originating from ZnTiO<sub>3</sub> with temperature change, as well as the relation between the crystal structures which have been predicted and the structure of the phases we have experimentally observed.

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