The Serbian Society for Ceramic Materials

Institute for Multidisciplinary Research, 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

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Branko Matović
Zorica Branković
Dušan Bućevac
Vladimir V. Srdić

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SPECIAL THANKS TO

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P-9

$BiFeO_3$ PEROVSKITES: THEORETICAL AND EXPERIMENTAL INVESTIGATIONS

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Bismuth ferrite ($BiFeO_3$) is one of the most studied multiferroic system. $BiFeO_3$ has been synthesized by controlled hydrothermal process, where the particles of small sizes and with high purity were obtained. Structural analysis showed that non-annealed powder can be perfectly fitted to rhombohedral space group *R3c* as α-$BiFeO_3$ phase. In addition, a structure prediction has been performed and 11 additional $BiFeO_3$ modifications have been proposed. In the next phase, an *ab initio* optimization of predicted structures has been performed and the structure of the γ-phase has been elucidated.

In addition, electronic and magnetic properties of $BiFeO_3$ were investigated using combination of experimental and theoretical methods. Theoretical studies were performed using a full potential linearized augmented plane-waves plus local orbital (FP(L)APW+lo) method, based on density functional theory (DFT). HRTEM analysis confirmed existence of twin stacking faults, which are responsible for enhanced magnetic properties. EPR measurements suggested existence of electrons trapped by vacancies or defects, while magnetic behavior of synthesized material was investigated by SQUID.