



**Serbian Ceramic Society Conference**  
**ADVANCED CERAMICS AND APPLICATION IX**  
**New Frontiers in Multifunctional Material Science and Processing**

**Serbian Ceramic Society**  
**Institute of Technical Sciences of SASA**  
**Institute for Testing of Materials**  
**Institute of Chemistry Technology and Metallurgy**  
**Institute for Technology of Nuclear and Other Raw Mineral Materials**

**PROGRAM AND THE BOOK OF ABSTRACTS**

**Serbian Academy of Sciences and Arts, Knez Mihailova 35**  
**Serbia, Belgrade, 20-21. September 2021.**

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### **Structural And Functional Investigation Of Fe/Pb/Zr-co-doped Barium Titanate Ceramics: From Theory To The Experiment**

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Mixtures of high purity powders of 50 mass% Fe, 4 mass% Pb, 3 mass% Zr and 43 mass% BaTiO<sub>3</sub> were activated in a rotary ball mill for durations ranging from 30 min to 300 min; samples were then sintered in the air atmosphere for 2 hours at 1200 °C. Crystal structure prediction has been performed using Bond Valence Calculation (BVC) method. Moreover, theoretical stability of the perovskite structure for synthesized and calculated Fe/Pb/Zr-co-doped barium titanate compounds has been investigated using the Goldschmidt tolerance factor (Gt) and global instability index (GII). It was observed that magnetization of the system decreased after the sintering, with the most dramatic drop of 90.11% belonging to the sample activated for 150 min. In comparison with initial powders, X-ray powder diffraction data confirmed the presence of new phases of BaFe<sub>12</sub>O<sub>19</sub> and Ba<sub>1.696</sub>Ti<sub>0.228</sub>O<sub>3</sub> in sintered samples. Utilizing the field emission scanning electron microscopy (FESEM), it was found that with the increase of activation time the morphology of the samples progressed from irregular, spherical grains to mostly rod-like ones. Energy dispersive X-ray (EDX) analysis identified the presence of Pb and Zr occupying the same locations on the surface of sintered samples, whilst Fe was uniformly deployed regardless of the activation time.