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
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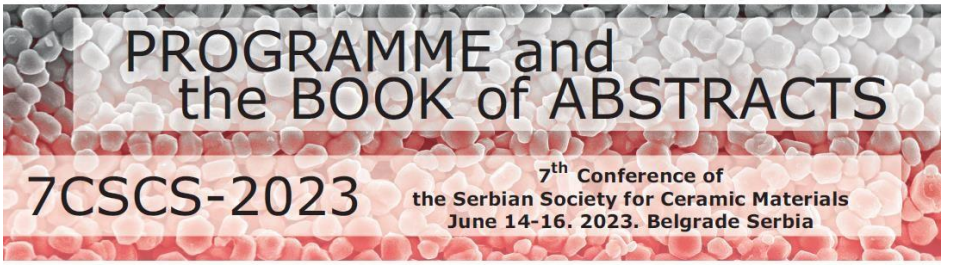

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Branko Matović
Jelena Maletaškić
Vladimir V. Srdić

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June 14-16, 2023
Belgrade, Serbia
7CSCS-2023

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SPECIAL THANKS TO

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ТЕХНОЛОШКОГ РАЗВОЈА И ИНОВАЦИЈА

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CRYSTALLOGRAPHIC INVESTIGATION OF THE IRON PHOSPHATE TUNGSTEN BRONZE (Fe-PWB

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In this paper, 12-tungstenphosphoric acid (PWA) was synthesized in combination with $FeCl_3$ at room temperature (25 °C). At such manner, Fe^{3+} ion exchange gave new 12-tungstenphosphoric salt of the transition metal iron ($FePW_{12}O_{40}\times nH_2O$; Fe-PWA). Thermal analysis determined the temperature of about 596 °C of the phase transition, i.e., the temperature at which the structure of the Kegin anion is disturbed. Therefore, it was chosen temperature above the breakdown of the Kegin anion of 650 °C, and which is required to obtain phosphate tungsten bronzes (PWB) doped with iron (Fe-PWB). The sample was kept in the oven for 10 min. Such obtained new Fe-PWB doped bronze was further investigated by the X-ray powder diffraction (XRPD) and Rietveld methods. The XRPD patterns of Fe-PWA and Fe-PWB were taken in the 3–90° 2θ angle range, and clearly reveal crystallographic and structural differences between these two phases. Determined unit-cell parameters of Fe-PWB obtained by the Rietveld method in the monoclinic crystallographic system are as following: a_0 = 7.53(2) Å; b_0 = 7.51(1) Å; c_0 = 7.64(1) Å; β_0 = 89.7(2)° and V_0 = 431(2) Å^3. These unit-cell parameters were compared with PWB, as well as other previously characterized doped bronzes (Li-PWB and Ca-PWB). It can be concluded that inserting of the Fe^{3+} ion into the PWB's structure was undoubtedly proven, and have the most influence to the axis a_0 (i.e. it significantly increased), angle β_0 (i.e., it significantly decreased), and volume V_0 (i.e., it significantly increased). On the other hand, influence to the axis c_0 is quite smaller (i.e. it slightly decreased), whereas influence to the axis b_0 is minor. Such behavior is also very different in comparison to the Li-PWB and Ca-PWB.