### SIXTEENTH ANNUAL CONFERENCE

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### STRUCTURAL INVESTIGATION OF $CaCu_3B_4O_{12}$ (B = Ti, Ru)

<u>Ljiljana Veselinović</u><sup>1</sup>, S. Marković<sup>1</sup>, M. Lukić<sup>1</sup>, L. Mančić<sup>1</sup>, S.D. Škapin<sup>2</sup>, M. Mitrić<sup>3</sup>, D. Uskoković<sup>1</sup>

Institute of Technical Sciences of SASA, Belgrade, Serbia, <sup>2</sup>Jožef Stefan Institute, Ljubljana, Slovenia, <sup>3</sup>Institute of Nuclear Sciences Vinča, University of Belgrade, Belgrade, Serbia

Perovskite-related materials with the general formula  $AC_3B_4O_{12}$  have great technological significance due to their specific physical properties. The crystal structure of  $AC_3B_4O_{12}$  compounds is cubic with  $Im \ 3$  symmetry. Different cations can occupy A and B sites, while the C site is commonly occupied by  $Cu^{2+}$  or  $Mn^{3+}$  ions. It has been found that the nature of B cation changes the physical properties of the material. In our previous studies we dealt with  $CaCu_3Ti_4O_{12}$  (CCTO) and  $CaCu_3Ru_4O_{12}$  (CCRO) compounds. CCTO has the gigantic permittivity of  $\sim 10^4 - 10^5$  in the kilohertz region and good stability over the temperature range from -170 to 330 °C. While Ti-compound is semiconductor, the Ru one is conductive oxide and could be used as interfaces between CCTO and metallic electrodes. Thus, CCTO and CCRO have potential application for preparation of layer capacitors with CCRO as the electrode and CCTO as the dielectric material. Since the oxygen vacancies and/or intrinsic defects in perovskites have a crucial role in the physical properties it is important to determine crystal structure of ceramic materials.

In this work, a detailed structural investigation of CCTO and CCRO perovskites was performed. The powders were prepared by precipitation and successive calcination at 1100 °C with 3 h dwell time to obtained single phased materials. The phase composition and crystal structure of synthesized powders were studied by X-ray powder diffraction (XRD), transmission electron microscopy (TEM), high-resolution TEM (HRTEM), selected-area electron diffraction (SAED) and Raman spectroscopy analyses. Rietveld refinement of XRD data was used to calculate the powders stoichiometry. Furthermore, since the XRD method is not adequate for determination of oxygen atoms due to their small scattering factors, to confirm the (oxygen-) stoichiometry of the ceramic powders, thermogravimetric (TG) measurements were employed. Two sets of experiments were performed; powders were heated in a flowing: (1) air atmosphere, and (2) reducing atmosphere (mixture of 5%  $H_2$  with Ar; 20 ml/min), to 1100 °C with a heating rate 10 °C/min with 3 h dwell time. TG measurements were performed on system coupled to a quadrupole mass spectrometer used for determination of volatile compounds. The weight losses measured by TG, in two different atmospheres, were compared; minor deviations in stoichiometries of  $CaCu_3B_4O_{12}$  compounds determined by Rietveld refinement were corrected.