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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Experimental and theoretical study of nanostructured $Ca_{1-x}Gd_xMnO_3$ (x=0.05; 0.1; 0.15; 0.2)

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Experimental and theoreticalmethodshave been used to investigate the octahedral tilting and related effects of $Ca_{1-x}Gd_xMnO_3$(x = 0.05; 0.1; 0.15; 0.2) compound. Both methods have shown that orthorhombic-perovskite structure (space group *Pnma*) is the most stable form and according to Glazer's classification belongs to $a^-b^+a^-$ tilt system. Bond valence calculations (BVC) have shown ten additional perovskite-related modifications of the equilibrium $Ca_{1-x}Gd_xMnO_3$structure, and their stability has been investigated as function of Gd doping. We have further studied the influence of gadolinium amount on Mn-O bond angles and distances, tilting of MnO_6octahedra around all three axes and deformation due to the presence of Jahn-Teller distortion around Mn^{3+}cation, and calculated the amount of Mn^{3+} in the system. BVCapproach is a simple, fast and efficient way of calculating the amount of Mn^{4+} and Mn^{3+} in the doped perovskite compound, which, to the best of our knowledge, has not been done before. The infrared reflection spectra of $Ca_{1-x}Gd_xMnO_3$samples confirmed XRD results that $Ca_{1-x}Gd_xMnO_3$nanopowders are of *Pnma*-1 structure and that the tilting of octahedra are increased with Gddoping. The EPR (electron paramagnetic resonance) spectra are in accordance with the assumption that EPR linewidth is Mn-O-Mn angle dependent. The studied samples showed that small octahedra tilting in these samples brought only a small change of the EPR linewidth.