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Effects of Sol-Gel Synthesis Procedure Conditions on the Stability of Polar Active Hexagonal Phase in $LuFeO_3$-$LuMnO_3$ System

A. Pakalniškis[1*], G. Niaura[2], D. Karpinsky[3], G. Rogez[4], P. Rabu[4], S. Chen[5,6], T. C-K Yang[5,6], R. Skaudžius[1], A. Kareiva[1]

[1] Institute of Chemistry, Vilnius University, Naugarduko 24, LT-03225 Vilnius, Lithuania
[2] Department of Organic Chemistry, FTMC, Sauletekio Ave. 3, LT-10257, Vilnius, Lithuania
[3]Namangan Engineering-Construction Institute, Dustlik Avenue 4, 160100 Namangan, Uzbekistan.
[4]IPCMS, 23 Rue du Loess Bâtiment 69, 67200, Strasbourg, France
[5]Precision Analysis and Materials Research Center, NTUT, Taipei, Taiwan
[6]Department of Chemical Engineering and Biotechnology, NTUT, Taipei Taiwan
andrius.pakalniskis@chgf.vu.lt

Nowadays the amount of extremely specific and niche applications is ever increasing. This is especially visible in the areas of electronic and magnetic materials. Because of this a lot of attention by scientist has been dedicated towards the invention of new materials or on the improvement of already existing ones in such a way as to adapt them for modern day requirements. One key area of research revolves around the combination different properties into a single material. While many of the different combinations have been attempted the merging of ferroic properties has attracted a lot of attention in particular. Currently compounds that exhibit at least two primary ferroic orders (elastic, magnetic or electric) are referred to as multiferroic [1].

However, the combination of both magnetic and electrical properties requires significant challenges to be overcome in order to be possible. Firstly, the classically know magnetic and electric properties arise from opposite phenomena. Since in most cases the ferroelectric properties arise from the hybridization of empty 3d orbitals and magnetic ones require them to be partially filled. In order to avoid encountering this problem other possible mechanisms for the existence of ferroelectricity were discovered. These mechanisms include lone pair, spin driven, geometric and charge ordering as they do not require empty electron shells [2]. Secondly, the coupling between the two is often weak. Lastly, at least one of the properties occurring at temperatures lower than that of room temperature. The solution to the last two problems is not as simple or clear and as in most cases is different for every material. As such the search for new multiferroic materials that would show both, ferroelectric and ferromagnetic properties with strong coupling and above room temperature is still ongoing.

Once such potential compound is hexagonal $LuFeO_3$. While undoped, $LuFeO_3$ is an orthorhombic non-polar perovskite with weak ferromagnetic properties. However, a metastable hexagonal crystal structure with $P6_3cm$ space group can be also obtained. The hexagonal variant of $LuFeO_3$ is a polar compound where ferroelectricity is caused by geometric factors, mainly the uneven displacement of Lu ions in the crystal structure [3]. The metastable structure can be stabilized by either strain during thin film preparation or by doping the $LuFeO_3$ matrix. While there are several different dopants possible their effects on magnetic properties and electrical properties are still not clear. Even the phase formation is complicated and the stability regions of the hexagonal phase are difficult to describe as they are different for each of the dopants while also being sensitive to the preparation method and even the calcination temperature [4].

As such in this work we provide insights into the stabilization of hexagonal $LuFeO_3$ by Mn doping prepared by aqueous sol-gel method. The concentration stability regions for the hexagonal phase at different calcination temperatures were described using X-ray diffraction analysis. Particle morphology was determined using SEM analysis. Lastly, we also provide additional information on the behavior of magnetic properties not only caused by the crystal structure changes, but also on the effect of Mn doping.

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