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TEMPERATURE DRIVEN PHASE TRANSITIONS IN METASTABLE Sc DOPED HEXAGONAL LuFeO₃

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The crystal structure and properties of compounds with perovskite structure (nominal chemical formula ABO₃) can be drastically modified by a chemical substitution in A- and/or B- perovskite sublattices. Introduction of elements with different ionic radii leads to a stabilization of structural distortions. The possibility to control physical properties via chemical doping is particularly important when concerning the formation of both electrical and magnetic orderings in the same compounds, which are commonly referred as multiferroics. However, for the most part, due to the conflicting nature of these properties, the coupling between the electrical and magnetic properties is relatively weak. Since magnetic properties usually require the 3d layer to be partially filled by electrons, while electrical properties arise from empty 3d shells. To solve this conundrum, materials with new mechanism for the origin of their ferroelectric properties were discovered, such as lone pair and spin driven mechanisms, that do not require empty electron shells [1]. The second issue that multiferroic compounds suffer from is the fact that most orderings only occur below room temperature. Only few room temperature multiferroics are known, with the main research being focused on BiFeO₃.

Recently a new class of hexagonal rare earth ferrite perovskite compounds has been found to exhibit multiferroic ordering, with a mechanism and structure similar to that of hexagonal manganites, making them a new avenue for potential research. This new family of room temperature multiferroic compounds are based on LuFeO₃ with hexagonal structure (space group *P6₃cm*). It has been discovered that LuFeO₃ in the hexagonal state has both ferroelectric and weak ferromagnetic ordering. Furthermore, it has been reported that the compound in orthorhombic phase (space group *Pnma*) is antiferromagnetic below 620 K, while being in hexagonal structure the magnetic transition shifts down to 440 K while also showing weak ferromagnetism, due to a canting of the magnetic moments towards the c-axis, with the polarization being retained up to 1050 K, at least in the case of thin films [2,3].

It should be noted, that the preparation of hexagonal compounds is quite difficult and the crystal structure can be modified either using the chemical substitution or via preparing the compounds in a form of thin films as the crystal lattice is unstable and tends to form an orthorhombic structure. Due to the unstable nature of the lattice and difficulty of preparation and characterization of the hexagonal variant of LuFeO₃, the main available results have been performed on thin films. However, when analyzing thin films, it is important to take into account the effect of strain and interface interactions as it can significantly affect chemical and physical properties [4].

We provide insights in stabilizing the hexagonal structure in doped LuFeO₃ polycrystalline compounds prepared using aqueous sol-gel synthesis procedure. While also providing further clarification on the concentration ranges of the different structural phases present in the system and analyzed by means of SEM, room temperature X-ray diffraction techniques, and Raman spectroscopy. Furthermore, we also investigate temperature driven polar to non polar phase transitions by means of temperature dependent X-ray diffraction measurements. Lastly, we provide additional insight on the magnetic structure and its changes at low and room temperature.

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