




Abstract

Crystal and Magnetic Structure Transitions in Doped Lu- and Fe-Based Perovskite Oxides [†]

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The possibility of controlling physical properties via chemical doping is particularly important when considering the formation of both electrical and magnetic orderings in the same compounds, which are commonly referred as multiferroics [1]. However, for the most part, due to the conflicting nature of these properties, the coupling between the electrical and magnetic properties is relatively weak. 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 is based on LuFeO₃ with a hexagonal structure (space group *P6₃cm*). It has been discovered that LuFeO₃ in its hexagonal state has both ferroelectric and weak ferromagnetic orderings [2,3]. As such, in this work, we adapted an ethylene glycol based sol-gel synthesis procedure for the preparation of bulk Sc doped hexagonal lutetium ferrite powders. The crystal structure was investigated using XRD and Raman spectroscopy at room temperature. The temperature-driven crystal structure transitions were analyzed by means of in situ high-temperature XRD while the magnetic transitions were investigated by means of low-temperature magnetization measurements. The obtained results revealed that at room temperature, the polar hexagonal phase can be stabilized in a quite narrow doping range that depends on the sintering temperature of the samples [4]. Additionally, samples with a higher Sc doping content showed a lower phase transition temperature from ferroelectric to paraelectric phases. While Sc itself is not magnetic, the Sc doping caused substantial changes to the magnetization of the samples as well. Overall, the results indicate that LuFeO₃ can be successfully synthesized by means of the ethylene glycol based sol-gel procedure. The desired phase composition, magnetic and electric properties can be optimized by means of the doping content and the sintering temperature.



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References

1. Fiebig, M.; Lottermoser, T.; Meier, D.; Trassin, M. The evolution of multiferroics. *Nat. Rev. Mater.* **2016**, *1*, 16046. [[CrossRef](#)]
2. Wang, W.; Zhao, J.; Wang, W.; Gai, Z.; Balke, N.; Chi, M.; Lee, H.N.; Tian, W.; Zhu, L.; Cheng, X.; et al. Room-temperature multiferroic hexagonal LuFeO₃ films. *Phys. Rev. Lett.* **2013**, *110*, 237601. [[CrossRef](#)] [[PubMed](#)]
3. Cao, S.; Zhang, X.; Paudel, T.R.; Sinha, K.; Wang, X.; Jiang, X.; Wang, W.; Brutsche, S.; Wang, J.; Ryan, P.J.; et al. On the structural origin of the single-ion magnetic anisotropy in LuFeO₃. *J. Phys. Condens. Matter* **2016**, *28*, 156001. [[CrossRef](#)] [[PubMed](#)]
4. Pakalniškis, A.; Alikin, D.O.; Turygin, A.P.; Zhaludkevich, A.L.; Silibin, M.V.; Zhaludkevich, D.V.; Niaura, G.; Zarkov, A.; Skaudžius, R.; Karpinsky, D.V.; et al. Crystal Structure and Concentration-Driven Phase Transitions in Lu_(1-x)Sc_xFeO₃ (0 ≤ x ≤ 1) Prepared by the Sol–Gel Method. *Materials* **2022**, *15*, 1048. [[CrossRef](#)] [[PubMed](#)]

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