

Structural and Physical Properties of the Double Layer Perovskite System ReBaFe₂O_{5+w} (Re=Rare Earth): Possible Application as Anode for Solid Oxide Fuel Cells - SOFC

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Abstract – We performed the synthesis of the double perovskite system REBaFe₂O_{5+w} (RE=Ce,La,Eu,Nd,Sm,Gd, and Y). For the first time CeBaFe₂O_{5+w} samples were synthesized. We followed a solid state preparation method to obtain all set of samples. Very pure single-phase samples having an orthorhombic crystalline structure (Pmmm space group) were obtained, as indicated by Rietveld analysis of X-ray diffraction data. Magnetization, ac susceptibility and heat capacity measurements were employed to characterize the magnetic properties. Our double layer perovskite system fill all features and is a promising material to be a SOFC anode.

In doped perovskite manganites, electron spins in the itinerant e_g band are aligned parallel to the localized t_{2g} spins due to strong Hund's rule coupling. Thus, conduction of spin-polarized e_g electrons results in ferromagnetic (F) nearest-neighbor interactions, known as double exchange (DE), or antiferromagnetic (AF) superexchange (SE) via localized t_{2g} electrons, in cooperative Jahn-Teller distortions. REBaFe₂O_{5+w} (RE=Nd–Ho and Y) double layer perovskites is a class of compounds where DE and SE interactions are in competition, resulting in either a charge ordered insulator or a mixed-valence conducting phase. In REBaFe₂O₅, DE occurs through the minority spin t_{2g} electrons that competes with AF-SE originated in the e_g bands. In this work, we performed the synthesis of the double perovskite system REBaFe₂O_{5+w} (RE=Ce,La,Eu,Nd,Sm,Gd, and Y). For the first time CeBaFe₂O_{5+w} samples were synthesized. We followed a solid state preparation method to obtain all set of samples. Very pure single-phase samples having an orthorhombic crystalline structure (Pmmm space group) were obtained, as indicated by Rietveld analysis of X-ray diffraction data. For the CeBaFe₂O_{5+w} sample, the room temperature lattice parameters are $a = 0.39646$ nm, $b = 0.39282$ nm and $c = 0.78285$ nm. Magnetization, ac susceptibility and heat capacity measurements were employed to fully characterize the magnetic properties. The CeBaFe₂O_{5+w} magnetic structure is characterized by the coupling of Fe atoms within double layers, and we found that the system orders ferromagnetically at $T_C \approx 600$ K. On cooling, the compound orders antiferromagnetically but remains valence-mixed. At $T_V \approx 129$ K, a Verwey-type transition orders the Fe valences and modifies the AF structure. Also, in this work, we will discuss the possible application of the double perovskites as an anode in a solid-oxide fuel cell (SOFC) for high temperature operation [1]. The solid oxide fuel cell is an electrochemical device that can be used for electrical energy generation from gaseous fuel. In a first moment, our double layer perovskite system fill all features [1,2] and is a promising material to be a SOFC anode that can operate with natural gas that is not so costly and is more convenient. We acknowledge the financial support from Brazilian science agencies CNPq and FAPESP.

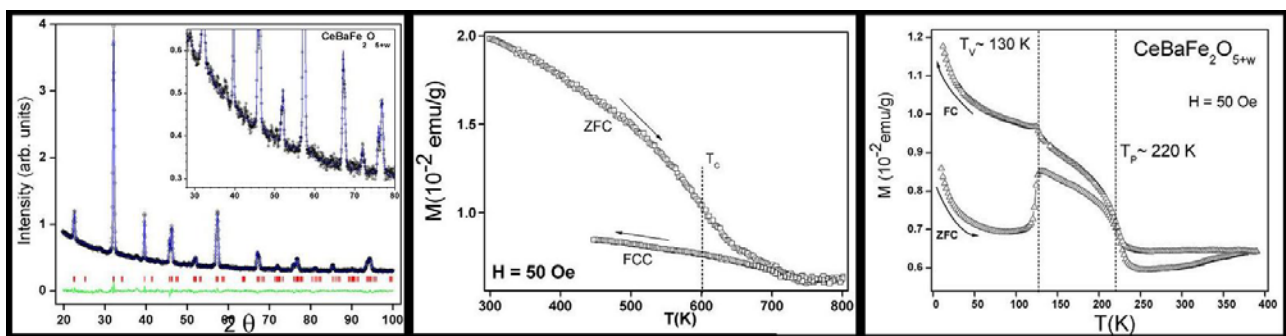


Figure 1: CeBaFe₂O_{5+w}: Pattern measured at room temperature with CuK_α radiation. Magnetization as a function of temperature (H = 50 Oe) showing a broad change around $T_C = 600$ K.

[1] Yun-Hui Huang, et. al., "Double Perovskites as Anode Materials for Solid-Oxide Fuel Cells" *Science*. 312, 254 (2006).

[2] R. Muccillo, E. N. S. Muccillo, F. C. Fonseca, et. al., "Development Testing of Anode-Supporte Solid Oxide Fuel Cells with Slurry-Coated Electrolyte and Cathode", *J. Power Sources*, 156, pp455 (2006).