Probing the role of (Gd-Co) co-doping on structural and thermal behavior of $LaFeO_3$

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Abstract: The structural and thermal behavior of sol-gel derived nanocrystalline $LaFeO_3$ (LFO) and $La_{0.7}Gd_{0.3}Fe_{0.7}Co_{0.3}O_3$ (LGFCO) has been investigated. The structure formation has been confirmed by the x-ray diffraction. LFO which is a distorted perovskite structure crystallizes in the orthorhombic structure with Pbnm space group. The distortion in the LFO system decreases with increase in temperature and becomes minimum at Neel point which is highest in LFO (740 K) [1]. However, above the Neel point distortions start to increase and the structure transforms to rhombohedral at 1220 K [2, 3]. Rietveld refinement is used for the analysis of x-ray diffraction data and is shown in Figure 1. The active vibrational bands around 410 cm^{-1} and 560 cm^{-1} in FTIR spectra [3, 4] (Figure 2) correspond to the two functional groups of the material which further validates the formation of samples. The vibrational bands in the doped sample are shifted towards higher wave-number which is persistent with the x-ray diffraction spectra. The shifting in the X-ray diffraction and FTIR spectra is due to the departure from the ideal $LaFeO_3$ sample on account of change in bond lengths and bond angles

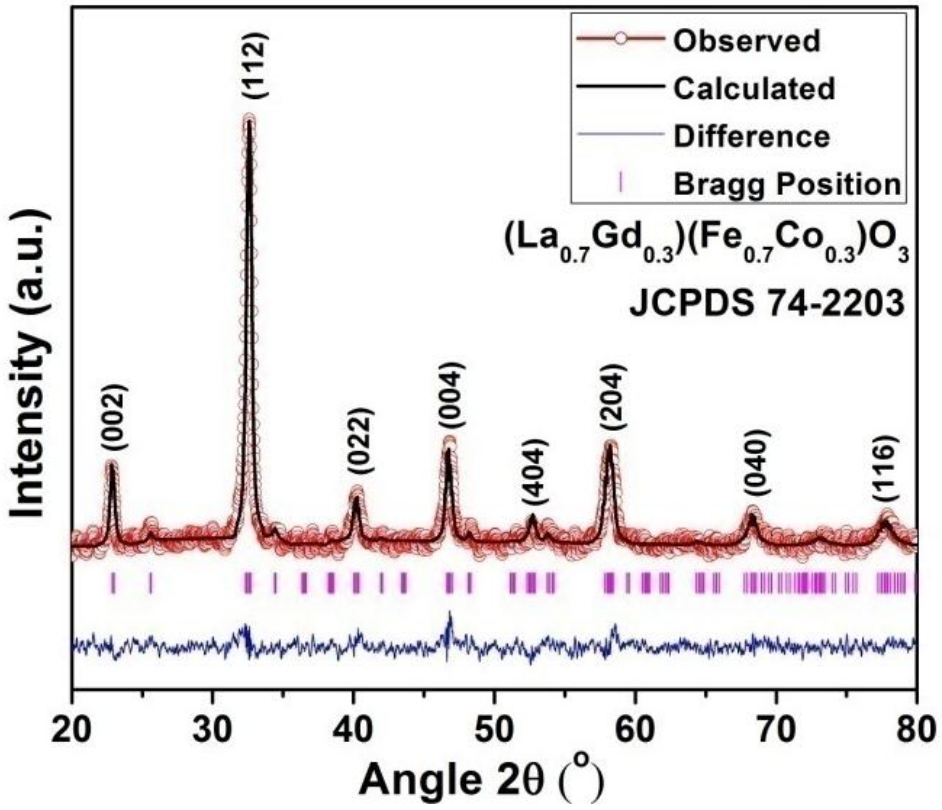

Figure 1: Rietveld refinement pattern of LGFCO sample.

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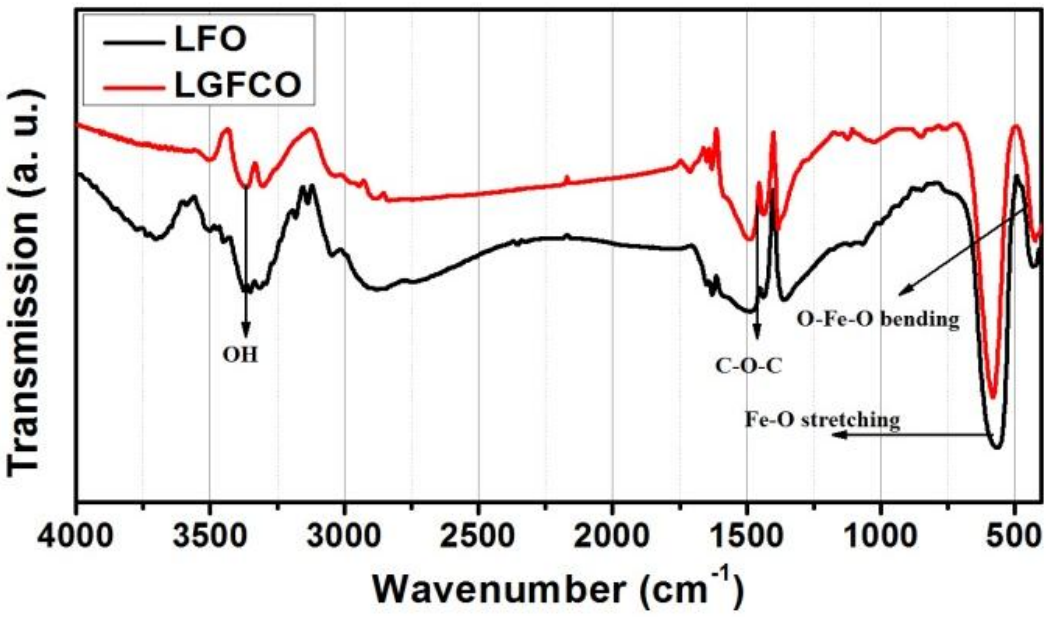

Figure 2: FTIR spectra of LFO and LGFCO samples.

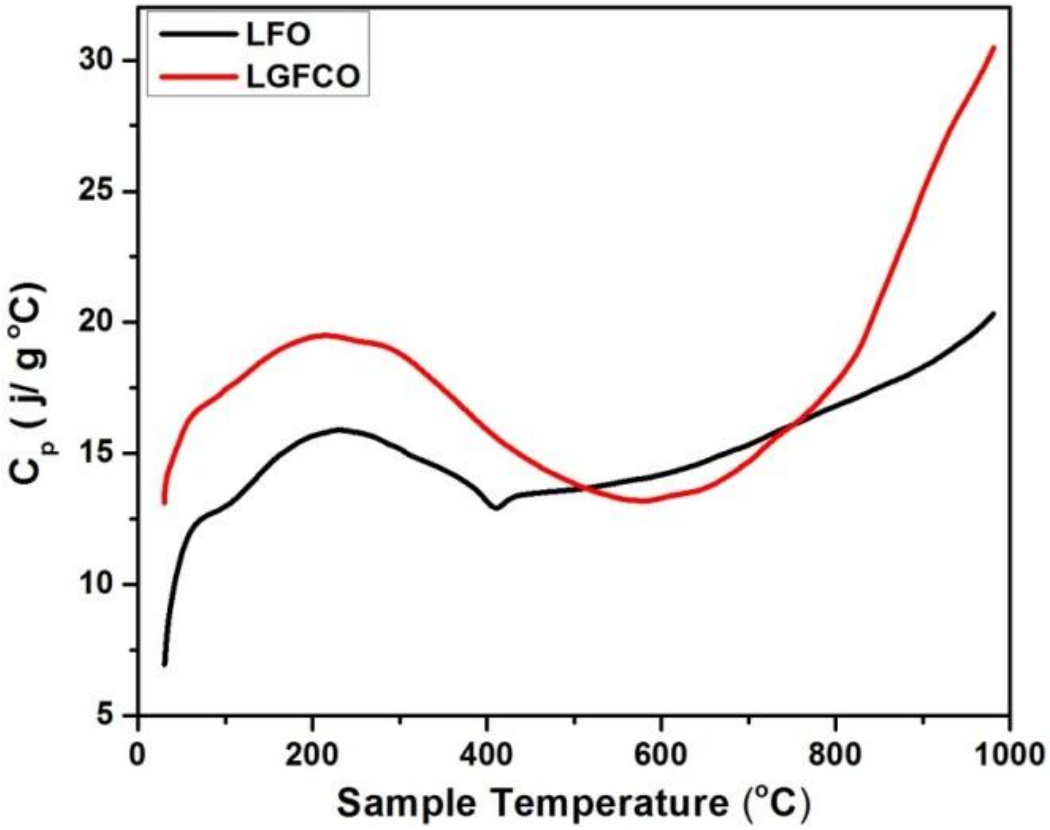

Figure 3: Specific heat variation against the sample temperature of LFO and LGFCO samples.

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To get an apprehension of high-temperature specific heat differential scanning calorimetry (DSC) has been performed using simultaneous thermal analyzer (STA) (Perkin Elmer). The variation of specific heat against temperature is shown in Fig.3 It has been observed from the specific heat plot LFO shows a small and sharp peak around antiferromagnetic Neel temperature however, the doped sample shows a broad peak around this point and above the Neel point specific heat increases.

At high-temperature above the Neel point the distortions in the system increase, spins are in paramagnetic state and the thermal energy supplied by increasing the temperature is utilized in providing the kinetic energy to the atoms and distorting the structure leading to an increase in the specific heat. However, the gradual decrease around Neel point in doped sample may be attributed to the different Neel points of the dopants

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