Comparative analysis of the structural, magnetic, dielectric and electrical properties of Ba^{2+} doped $PrFeO_3$ through solid-state and sol-gel auto- combustion routes

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Abstract

In the present study, we synthesized $Pr_{1-x}Ba_xFeO_3$ where x= 0.1, 0.2, 0.3 through solid-state and sol-gel auto- combustion routes. Firstly, we theoretically calculate the Goldschmidt tolerance factor (T) of perovskite compounds $Pr_{1-x}Ba_xFeO_3$ and found T lies between 0.71 - 0.9, so the already predicted structure from theoretical calculation is Orthorhombic. Further, the comparative structural, magnetic, and dielectric and electrical properties was studied using an X-ray Diffractometer (XRD), Vibrating Sample Magnetometer (VSM), and Impedance Analyzer and Two-probe set with oven respectively. XRD confirms the orthorhombic phase of $PrFeO_3$ with space group Pbnm and matches with PDF no.98-002-0768. $PrFeO_3$ is an antiferromagnetic but there is some weak ferromagnetism arise in samples formed by sol-gel due to Dzya-loshinskii-Moriya (DM interaction). From ac conductivity fitting plot we found the fitting parameter n lies below 1 (i.e. n<1) that means translation hopping is assisted by small polaron hopping mechanism. The resistivity versus temperature plot indicates that as temperature increases, resistivity decreases from an initial value of 10^3 ohms, which is characteristic of semiconductors. Resistivity of samples formed by solid state has lower resistivity than samples formed by sol-gel route due to higher surface to volume ratio of nanoparticles.

Introduction

Praseodymium orthoferrite ($PrFeO_3$) is a perovskite-type material that has garnered significant interest due to its versatile structural, magnetic, electrical, and dielectric properties. These characteristics make $PrFeO_3$ a promising candidate for various technological applications, including sensors, catalysts, magnetic devices, and electronic components[1,2]. Understanding the factors that influence these properties is crucial for optimizing the material's performance for specific applications. One such influential factor is the particle size. Recent advancements in nanotechnology and materials science have enabled the synthesis of $PrFeO_3$ particles with controlled sizes, ranging from bulk to nanometer scales. The particle size can profoundly impact the material's properties due to the increased surface-to-volume ratio, surface energy, and quantum confinement effects in smaller particles[3]. This study aims to systematically investigate the impact of particle size on the structural, magnetic, electrical, and dielectric properties of $PrFeO_3$. By synthesizing $PrFeO_3$ particles of varying sizes and characterizing their properties using a range of analytical techniques, we seek to elucidate the underlying mechanisms driving these

Applications

Magnetic Materials | Catalysts | Fuel Cells | Thermoelectric Materials | Dielectric Materials | Multiferroic Materials | Optoelectronic Devices

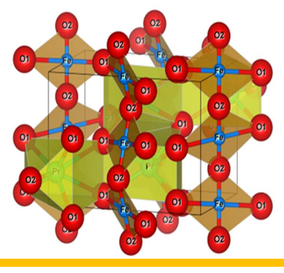
Structural Information using VESTA Software

In one unit cell

Total no. of atoms= 70

Total no. of Fe-O, Pr-O bonds= 104

Total no. of polyhedral= 16



Goldschmidt tolerance factor (*T*)

The concept of the tolerance factor can be extended to perovskites with more complex compositions by using an average value for ionic radii or bond length . For example, for an A-site substituted phase $A_{1-x}A'_xBX_3$, one can write

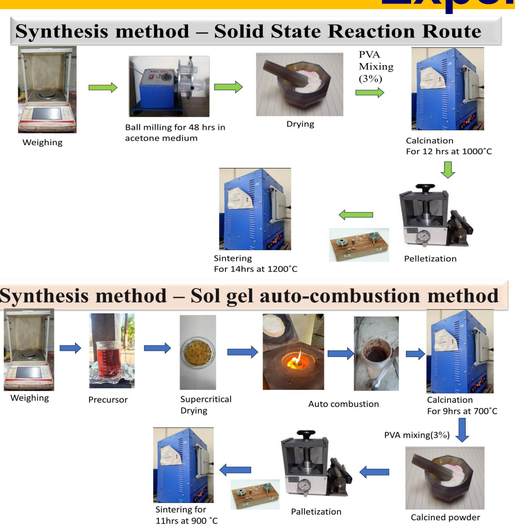
$$t = \frac{[\,(1-x)r_A + xr_{A'} + r_X\,]}{\sqrt{2}(r_B + r_X)}$$

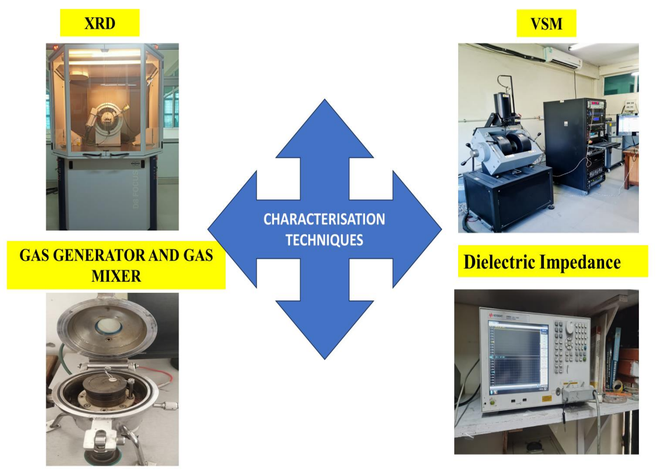
Goldschmidt tolerance factor (t)	Structure
>1	Hexagonal or Tetragonal
0.9-1	Cubic
0.71 - 0.9	Orthorhombic or Rhombohedral
0.71	Different Structures

Doping concentration	Sample Name	Tolerance Factor
x = 0.0	$PrFeO_3$	0.817
x = 0.1	$Pr_{0.9}Ba_{0.1}FeO_3$	0.827
x = 0.2	$Pr_{0.8}Ba_{0.2}FeO_3$	0.836
x = 0.3	$Pr_{0.7}Ba_{0.3}FeO_3$	0.846

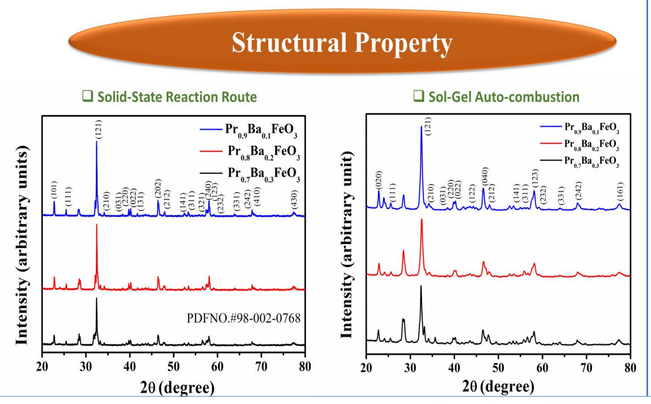
- As tolerance factor *t*, lies between 0.71 - 0.9, so the already predicted structure from theoretical calculation is either Orthorhombic or Rhombohedral.
- As doping increase from *x*=0.1 to *x*=0.3 , the structure approaches toward ideal cubic perovskite structure in both series.

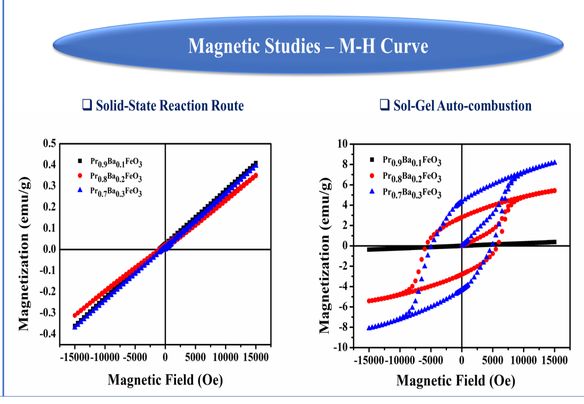
Experimental Set up

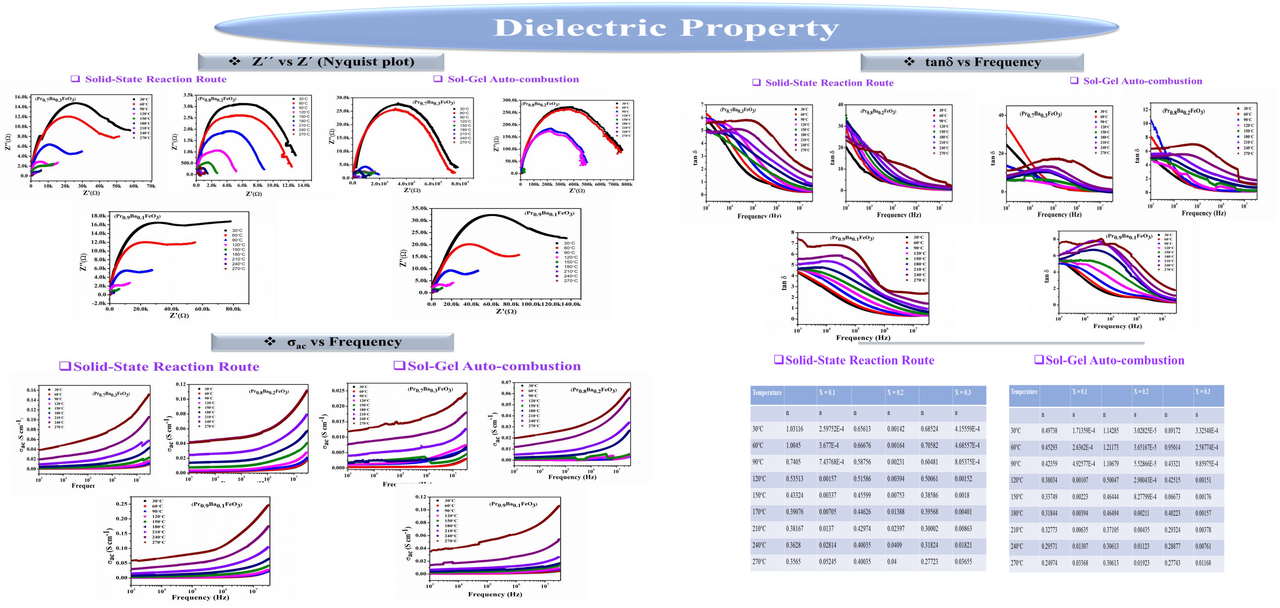


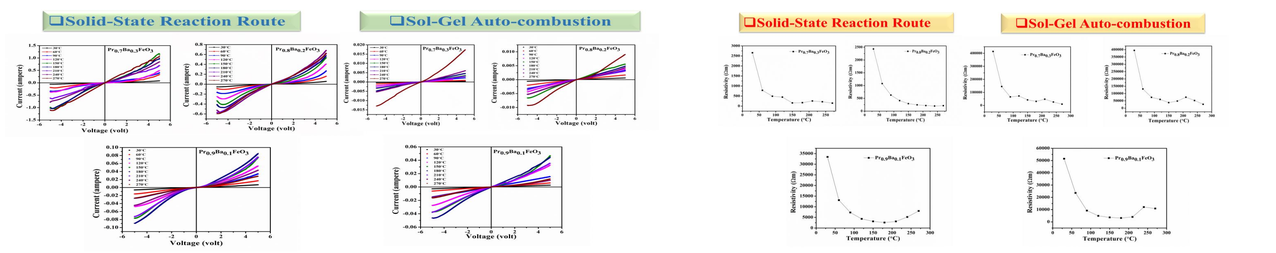


Results









Conclusions

The XRD results show that $PrFeO_3$ are having orthorhombic structure and space group P b n m with space group number 62. The weak ferromagnetism arise in samples prepared by auto-combustion method is due to Dzya-loshinskii-Moriya (DM interaction). The value of Z'' decreases with rise in temperature as well as frequency which reveals the reduction of resistive properties in the sample. A significant broadening of the peaks with rise in the temperature ensures the temperature-dependent electrical relaxation phenomenon in the material. The relaxation process may possibly be due to immobile species/electrons at lower temperatures and defects/vacancies at higher temperature. Peaks observed in the plots of tanδ as a function of frequency at various temperatures for x=0.1,0.2,0.3 samples indicating the existence of relaxation mechanism. The shifting of peaks towards higher frequency with rise in temperature, thereby suggests the relaxation to be thermally activated process. n increases with rise in temperature for x=0.1,0.2,0.3 samples and value of n lies below 1 (i.e. n<1) means that translation hopping is assisted by small polaron hopping mechanism. Resistivity of samples formed by solid state has lower resistivity than samples formed by sol-gel route due to higher surface to volume ratio of nanoparticles.

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