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Structural distortion, ferroelectricity and ferromagnetism in $Pb(Ti_{1-x}Fe_x)O_3$

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ABSTRACT: Recently interest in finding magnetoelectric coupling in *Fe* substituted $PbTiO_3$ is observed. Synthesis of single phase $PbTi_{(1-x)}Fe_{(x)}O_3$ is a challenge which we report for $0 \leq x \leq 0.5$. $PbTiO_3$ is a strong ferroelectric. Fe substitution at the *Ti* site may lead to a potential magnetoelectric multiferroic material maintaining the non-centrosymmetric lattice distortion due to elongation of *Ti-O* octahedral in $PbTiO_3$ intact. The synthesis chemistry is a determining factor on the pure phase. Valence state, size and coordination of substituting *Fe* is a determining factor of how the lattice distortion will get modified deciding several changes including oxygen deficiency, *etc*., and results in variations of electronic/magnetic properties including ferroelectricity and magnetism. We investigate the structural and electronic properties and correlate discussing briefly the introduced magnetic properties and subsequent structural changes linked to ferroelectricity.

Keywords: $PbTiO_3$, Ferroelectricity. Ferromagnetism.

Introduction

$PbTiO_3$ and other perovskite titanates are recognized for their ferroelectric behavior which undergoes structural phase transitions.[1] Amongst the perovskite titanates, $PbTiO_3$ is one of the strongest ferroelectric materials, with a high pyroelectric coefficient, a high spontaneous polarization and a high Curie temperature. It is a ferroelectric ceramic used in capacitors, ultrasonic transducers, thermistors, optoelectronics and pyroelectric infrared detector applications.[2] The tetragonality of $PbTiO_3$ is a signature of enhanced ferroelectric properties and is measured by the *c/a* ratio which in pure $PbTiO_3$ is ~1.06 at room temperature [3] and is considerably higher than other perovskite titanates. The ratio decreases with increasing temperature and finally at ~490^{o}C the tetragonal phase changes to a cubic phase.[2]

There are many reports of substituted $PbTiO_3$ series such as $PbZr_{(x)}Ti_{(1-x)}O_3$ (PZT) [4], $Pb_{(x)}Ca_{(1-x)}TiO_3$ [5], $Pb(Zn_{1/3}Nb_{2/3})O_3$-(x)$PbTiO_3$(PZN-PT) [6] and $Pb(Mg_{1/3}Nb_{2/3})O_3$-(x)$PbTiO_3$ (PMN-PT) [7] in which certain functionalities are enhanced. One such functionality is in the field of magnetoelectric multiferroics where magnetic ions are used in place of *Ti* and *Pb* ions to generate magnetism. $PbTi_{(1-x)}Fe_{(x)}O_3$ is one of the most important member of this group. The interest in this material has increased since Palkar *et al*.[8] showed magnetoelectric coupling using *MFM/EFM* studies. However, certain phase related questions to the actual origin of the magnetism exist. A detailed electronic