Chapter 6
Summary and Future scope

Megha U. “Synthesis and studies of nanostructured thermoelectric perovskite materials”
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Chapter 6
Summary and Future Scope

6.1 The present work

Rare earth cobaltates are potential candidate for thermoelectric applications. The method of synthesis, characterization and thermoelectric studies on rare earth cobalt iron oxide based perovskites are performed in the present work.

The aim of the present study was to synthesis Bi and Sr doped RCo_{0.6}Fe_{0.4}O_3 (R–La, Pr, Nd) by citrate-sol gel auto-combustion method and investigated the studies on structural, electronic, electrical, magnetic and thermoelectric properties. The substitution of Bi (x=0.1) in R-site enhances the thermoelectric properties of the sample. The power factor (PF), which determines the performance of the thermoelectric material get enhanced by replacing La by Pr and Nd. It is observed that, high value of PF is obtained for Nd_{0.9}Bi_{0.1}Co_{0.6}Fe_{0.4}O_3 (N1) and is found to be more suitable candidate for thermoelectric applications.

6.2 Summary of results and conclusions from the present thesis work.

The effect of Bi and Sr doping on the structural, electronic, electrical, magnetic and thermoelectric properties of Bi and Sr doped RCo_{0.6}Fe_{0.4}O_3 (R – La, Pr, Nd) have been studied using X-ray diffractometer (XRD), Scanning electron microscopy (SEM), Energy dispersive X-ray analysis (EDAX), X-ray photoelectron spectroscopy (XPS), particle size analyser, Impedance spectrometer, LCR-meter, Vibrating sample magnetometer (VSM), Physical property measurement set up (PPMS) and finally the dc electrical conductivity and Seebeck coefficient is measured by SEM-3 thermoelectric measurement set up. The studies are summarised in Table. 6.1
<table>
<thead>
<tr>
<th>Studies</th>
<th>Bi &amp; Sr doped LaCo_{0.6}Fe_{0.4}O_{3}</th>
<th>Bi &amp; Sr doped PrCo_{0.6}Fe_{0.4}O_{3}</th>
<th>Bi &amp; Sr doped NdCo_{0.6}Fe_{0.4}O_{3}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crystal Structure</td>
<td>Rhombohedral crystal structure with R3c space group, Bi (x=0.2) has the presence of secondary peaks, Strain value is in the order of 10^{-3} from the W-H plot.</td>
<td>Orthorhombic crystal structure with pbnm space group, Bi (x=0.2) has the presence of secondary peaks, Strain value is in the order of 10^{-3} from the W-H plot.</td>
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<tr>
<td>SEM images (Average grain size)</td>
<td>200-400 nm, decreases with doping of Bi and Sr</td>
<td>300-400 nm, decreases with doping of Bi and Sr</td>
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<tr>
<td>Particle size analyser (Size)</td>
<td>200-400nm</td>
<td>300-400nm</td>
<td>200-400nm</td>
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<tr>
<td>EDAX spectra</td>
<td>Confirms the elemental composition</td>
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<tr>
<td>XPS (oxidation states)</td>
<td>La, Bi, Co, Fe - +3, Sr - +2, satellite peaks are present in Co and Fe spectra, Only slight shift in B.E by doping, compounds have similar perovskite structures, L3 has large value of O_{A}/O_{L} indicates large number of oxygen vacancies.</td>
<td>Pr, Bi, Co, Fe - +3, Sr - +2, satellite peaks are present in Co and Fe spectra, Only slight shift in B.E by doping, compounds have similar perovskite structures, P3 has large value of O_{A}/O_{L} indicates large number of oxygen vacancies.</td>
<td>Nd, Bi, Co, Fe - +3, Sr - +2, satellite peaks are present in Co and Fe spectra, Only slight shift in B.E by doping, compounds have similar perovskite structures, N3 has large value of O_{A}/O_{L} indicates large number of oxygen vacancies.</td>
</tr>
<tr>
<td>Impedance studies at room temperature</td>
<td>semicircular Cole-Cole for L0, L1 and L2, L3 has no impedance, L2 has large value of impedance due to the secondary peak of Bi, presence of relaxation, grain boundary effect dominates</td>
<td>Similar behaviour is obtained and the value of impedance obtained is higher than L-series due to the presence of 4f electron shielding of Pr</td>
<td>Similar behaviour is obtained and the value of impedance obtained is higher than L-series and P-series due to the presence of 4f electron shielding of Nd</td>
</tr>
</tbody>
</table>
### Dielectric studies at room temperature

Dielectric constant as well as loss coefficient decrease with increasing frequency, L1 has large value of tanδ, L3 has large conductivity and L2 has less conductivity due to the secondary peaks of Bi, the process of relaxation is well explained by Maxwell-Wagner model.

Similar behaviour is observed

Similar behaviour is observed

### Magnetic studies

L0 has the presence of phase transition and is suppressed by the substitution of Bi and Sr doping. L2 has large magnetization due to the presence of secondary peaks of Bi

No phase transitions and the magnetization is decreased by the doping of Bi and Sr.

Existence of cusp due to the domain pinning effect and is suppressed by doping Sr.

### DC electrical conductivity

Semiconducting nature, Electrical conductivity increases by doping of Bi and Sr. L3 has high conductivity.

Similar behaviour is noticed and the conductivity is higher than L-series.

Similar behaviour is noticed and the conductivity is higher than L-series and P-series.

### Seebeck coefficient

Positive value, p-type thermoelectric generators.

Positive value, p-type thermoelectric generators, lesser than L-series due to degeneracy of 4f electron of Pr

Positive value, p-type thermoelectric generators, lesser than L-series and P-series due to degeneracy of 4f electron of Nd.

### High Power factor

L1 \( (1.460 \times 10^{-5} \text{ Wm}^{-1} \text{ K}^{-2} \text{ at } 380^0 \text{ C}) \)

P1 \( (2.466 \times 10^{-5} \text{ Wm}^{-1} \text{ K}^{-2} \text{ at } 380^0 \text{ C}) \)

N1 \( (3.197 \times 10^{-5} \text{ Wm}^{-1} \text{ K}^{-2} \text{ at } 380^0 \text{ C}) \)

### Jonker Analysis

Good agreement

Good agreement

Good agreement
6.3 Future Scope

There is ample scope for the further investigation on these samples, as they are potential candidate for thermoelectric materials. A complete investigation of all aspects requires high level equipments and it is time consuming. However, they are not included in the present investigation. Even at this level, one can convincingly predict the scope of thermoelectric materials for device applications. The dc electrical conductivity and Seebeck coefficient measurements is carried out for all samples and inorder to complete the thermoelectric studies one has to perform the thermal conductivity measurements. The thermal conductivity has to be measured to find the efficiency of these materials for thermoelectric applications. The dimensions of these materials can be further reduced by choosing different chemical routes such as hydrothermal method, precipitation from homogenous solutions etc. which are expected to show better thermoelectric properties. The size dependent thermoelectric properties of these materials have to be studied. The thin films of the samples can be made using sputter deposition or pulsed laser deposition and the properties have to be studied. Thermoelectric measurements in various ranges of temperatures have to be studied.