Chapter-6

Conclusions and Future Scopes

CHAPTER 6: Conclusions and Future Scopes

6.1 Conclusion of the Present Investigation

In overall thesis work, it has been concluded that lanthanum silicate is a cost effective and high oxide ion conducting electrolyte material for solid oxide fuel cell. We have studied structural, microstructural and thermal properties of the investigated system and established a correlation between the critical angle and electrical conductivity. We have also concluded that with the doping of alkaline earth metal we can enhance its ionic conductivity. Now, based on the results summary of the present work is as follows:

- The apatite type single phase $La_{9.67}Si_6O_{26.5}$ compound with hexagonal structure having space group $P6_3/m$ is synthesized.
- Conductivity spectroscopic technique shows that conduction is due to mainly mobile oxide ions. Dimensionality has been calculated based on Jonscher's power law exponent factor and it was found the predominantly one-dimensional migration of oxide ion through the interstitials. This was further confirmed by the bond balance energy landscape analysis of the system.
- The alteration of La site with different ionic radii has been done to form $(La_{1-x}A_x)_{9.67}(Si\ O_4)_6O_{2+\delta}(x = 0.0,0.05,0.10,0.15)$ where A=Ca and Ba. The ionic radii of substituents have altered the average area of critical triangle (saddle point).

- With ionic radii variation, ion mobility volume has risen to nearly 3 times in Ca substituted sample than Ba substituted sample. We have obtained La deficient Ca substituted samples and O deficient Ba substituted samples.
- The conduction is occurring via overlapping large polaron tunnelling and the potential barrier is generated by the excess oxide ions that can show long range diffusion in the ab-plane through interstitials and La2 vacancy creation.
- This hopping of oxygen is governed between the localized states generated between La vacancies and oxygen content as the interatomic spacing is higher than La1-O3 bond lengths for the samples. Further, the polaron radii reduce with Ca substitution and larger the polaron radius, higher will be the frequency exponent. This is showing the overlap of potential wells of the neighbouring sites (occupied and unoccupied sites) because of long range Coulomb interaction.
- Thus, with the creation of La -vacancies, hopping energy is reduced for x = 0.1. We found that for x = 0.0, scattering coefficient (SC) due to optical phonon scattering is reduced to 1/2 while acoustic phonon scattering is reduced to nearly 1/4 for x = 0.1.
- This study suggests that in apatite structure, ion conduction can be enhanced due to large polaron formation via phonon amplitude enhancement.

6.2 Scope for Future Work (New Directions and Future Perspectives)

The intriguing properties of electrolyte materials like microstructure, density, thermal and electrical compatibility for solid oxide fuel cells (SOFCs) depend on their synthesis route, dopants concentrations and microstructures. In this context, to achieve good conductivity and better performance of the materials, these parameters must be optimized. The microstructure is quite sensitive to the processing parameters such as sintering temperature, atmosphere used during sintering, processing routes and the amount of extra phase infiltration. So, a detailed study on the effect of these processing parameters on the structural, microstructural, thermal and electrical properties of the investigated compositions is required. Therefore, the structure-property correlation reveals the deep insights to understand the influence of oxygen ion conductivity with A and B site doping of proposed perovskite electrolyte systems.

One important direction is to exploit the novel exotic electrolyte system from a simple, robust and cost-effective chemical method in order to transcend some of the difficulties facing materials development for low and intermediate temperature SOFCs. Although vigorous efforts are made to experimentally characterize ionic diffusion and to develop optimal electrolytes through structure-property correlation, experimental studies do not lend to an understanding of the mechanism of ionic conduction at the atomic level. Another important new direction is to develop a predictive (density functional theory (DFT)) computational framework by carefully designed experiments, for the rational design of better electrolyte materials and structures for a new generation of SOFCs. This understanding is important in order to develop better ionic conductors. Therefore, the

thrust of area is to develop a fundamental understanding of oxygen vacancy migration at the atomic level for apatite based and other electrolyte systems. Therefore, the keeping above view the following points are considered for the future prospect in these regimes:

1. Some of the novel and exotic electrolyte system should be developed which can have optimized ionic conductivity and may be considered in perspective of chemical and thermal stability and most importantly their operation at low or intermediate temperature range.

2. The conductivity behavior of the sample at different partial pressure of oxygen should be studied to know the pressure range in which the conductivity is purely ionic.

3. The transference number is one of the important factors to predict the nature of the conductivity of electrolyte samples.

4. A fine and excellent quality of tape should be fabricated using tape casting method for optimized ionic conductivity of electrolyte systems by proper optimization of slip rheology using appropriated wt% of dispersant, solvent, binder, plasticizer and de-foamer.

5. The performance of the optimized electrolyte systems may be checked their compatible with anodes and cathodes.

6. Measurement of thermal expansion coefficient will be useful to study the compatibility of these electrolytes with the other component of cells.

7. Tape of bilayer composite electrolyte film should be formed to enhance the ionic conductivity as well as reduce the operating temperature that can be feasible for low and intermediate temperature SOFCs.

8. A theoretical investigation of the ionic conductivity is important that should be carried out using DFT calculations because it can be used to explore how dopant types and dopant concentrations influence the ionic conduction and to understand the mechanisms of diffusion in doped electrolyte systems.